

AN INTERACTIVE WEB ACCESSIBLE GAMMA-SPECTRUM SIMULATOR

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ABSTRACT

A versatile γ -spectrum simulation tool has been developed to allow the generation of accurate γ -spectra for a wide range of NaI and HPGe detectors and for any mixture of γ -emitting radionuclides. The simulator provides full interactive control of a virtual γ -spectrometer for modeling various geometries with shielded and unshielded sources. The output consists of an interactive graph, containing cumulative and nuclide specific spectral distributions. More detailed spectral information and a detection efficiency graph are available as advanced options. The simulator, which can be accessed through the NUCLEONICA nuclear science and data portal, is a powerful tool for providing basic and advanced training in various areas of nuclear science and applications.

1. Introduction

Nowadays the γ -spectrometry is used on a daily basis in different basic and applied fields of nuclear science and technology. A variety of instruments and measurement techniques, involving γ -spectrometry measurements, are employed routinely by nuclear and radio-chemists, health physicists, nuclear facility operators, radiation protection staff, safeguards inspectors, border police, customs and law-enforcement officers. Needs for education and training in these areas are high and, obviously, they will be increasing in the future as new challenges, such as strengthening nuclear safeguards and security, nuclear terrorism prevention and implementation of new standards in radiation safety and protection, arise. Contemporary web technologies coupled with advanced mathematical simulation can offer unique possibilities to address these growing demands by providing realistic visual interactive web-accessible teaching aids and tools. This paper reports on the first stage of the development of such a realistic web-based simulation tool, the Gamma Spectrum Generator, which can be accessed through the NUCLEONICA [1] nuclear science and data portal at www.nucleonica.net.

2. Basics of the simulation approach

The current implementation of a virtual measurement setup is based on a point-like γ -ray source located on the axis of a cylindrically symmetric NaI or High-Pure Ge (HPGe) crystal (the sensitive volume of a γ -spectrometer) and separated from it by a number of absorbing layers, as shown in Fig.1. The γ -spectrum for such measurement setups is constructed by summing appropriately normalized detector response profiles, generated for individual γ -rays emitted by a source.

The response profiles consist of peak and continuum components. The former includes the full energy peak (FEP), single and double escape peaks (SEP and DEP), X-ray escape peaks (XEP), and the 511 keV annihilation peak. The continuum component contains two contributions, both coming from Compton scattering events, which occur either inside a detector crystal or its surroundings. Although it is continuous in nature, the latter is often referred as a backscatter peak.

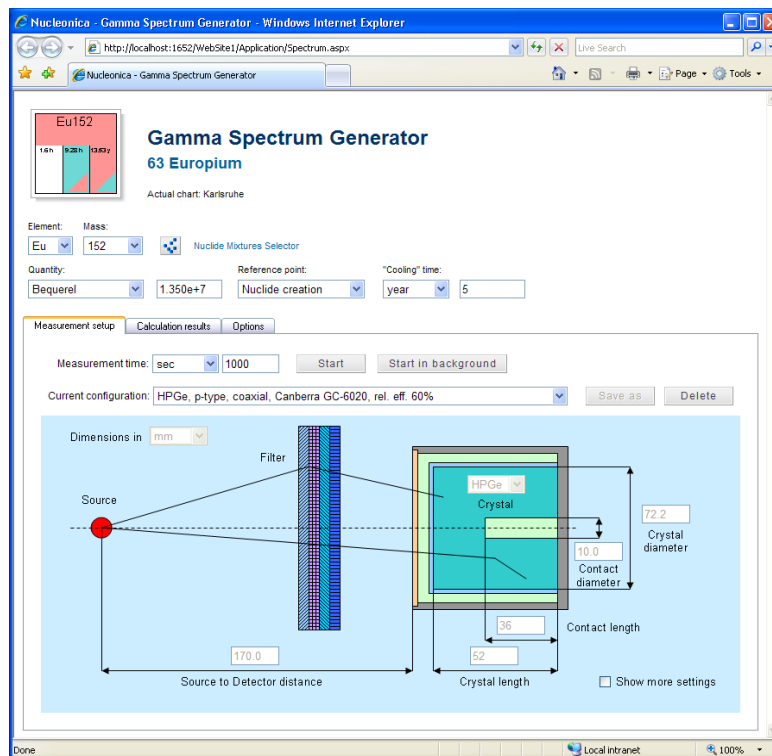


Fig 1. A screen capture of NUCLEONICA's Gamma Spectrum Generator web-page showing a tab with basic measurement geometry setup controls.

The relative contributions of the spectrum components are evaluated using an extensive detector response database, which has been created with help of a specially developed and validated Monte Carlo program. The database contains a large set of the peak-to-total and continuum-to-total efficiency ratios, and parameterized continuum shapes, calculated on grids of detector crystal dimensions, γ -ray energies and source-to-detector distances. In the course of modeling, a set of special interpolation techniques [2] is applied to calculate the efficiency ratios and continuum profiles for an arbitrary measurement setup and photon energy. Gaussian and Voigt distributions are used to model shapes of γ - and X-ray peaks, respectively. The peak widths represent actual energy resolution of a detector with additional contributions from Doppler broadening and natural line widths.

Once the relative response profile is constructed, it is converted to absolute values by performing normalization to the total detection efficiency. This efficiency is calculated by numerical integration over a detector crystal volume for the specified location of a source. The final response normalization is performed to account for the emission probability of particular γ -ray and actual number of decays of a respective nuclide, occurred during spectrum measurement. The latter is calculated based on the extended Bateman's analytical solution [3] of the system of differential equations governing radionuclide buildup and decay during source cooling and spectrum measurement time intervals.

Evaluated reference nuclear decay and photon attenuation data available in NUCLEONICA are used throughout spectrum modeling.

3. Features implemented

Fig.1 shows main features implemented in Gamma Spectrum Generator web-page. Using respective controls, an arbitrary individual nuclide or a pre-defined mixture of nuclides can be selected as a radiation source. A nuclide or a mixture of interest may be chosen also from NUCLEONICA's Nuclide Explorer or Nuclide Mixtures pages, which can be reached using corresponding links. Once a source nuclide is selected, the box at the top left of the page shows an image with its basic properties (decay modes, half-live, existing isomers) indicated. The nuclide's name to the right of the image provides a link to a part of the NUCLEONICA

Wiki, which describes in detail properties of the chemical element. The quantity (activity, mass or number of atoms) of a nuclide or a mixture can be specified either at the moment of its production/certification or at the spectrum measurement starting point of time. In the former case controls for specifying duration of a source cooling time interval become available.

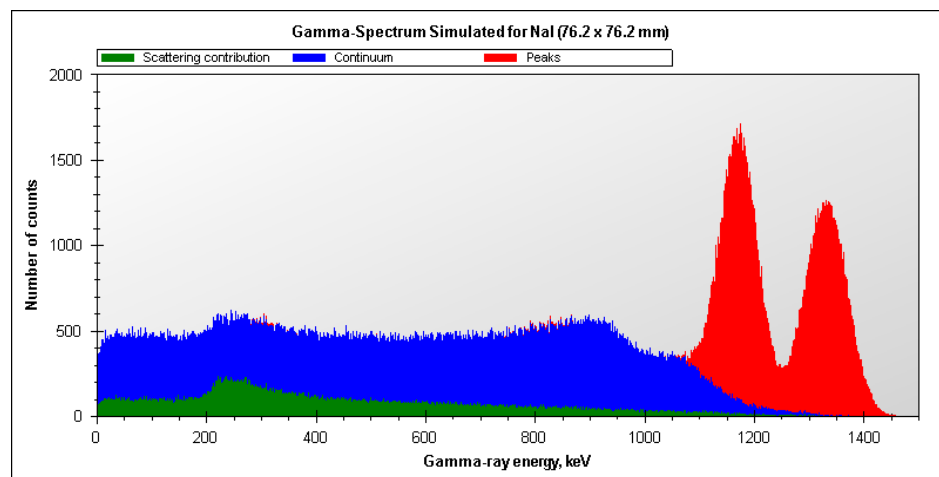
The spectrum measurement time and γ -spectrometer parameters can be specified on "Measurement setup" tab. Using the "Current configuration" dropdown list, one can choose a suitable γ -spectrometer from 6 pre-defined configurations, which include 2 coaxial HPGe detectors with 50% and 150% relative efficiency, low-energy (LEGe) and broad-energy (BEGe) HPGe detectors, and 2 scintillation detectors with standard $\varnothing 3'' \times 3''$ and $\varnothing 2'' \times 1''$ NaI crystals. The last entry ("Edit") in the drop-down list switches controls on the underlying measurement setup to the edit mode, whereby one can configure his own γ -spectrometer. The configurable parameters include the source-to-detector distance, as well as dimensions and materials of the detector construction elements, such as the detector crystal, crystal reflector, crystal packaging, crystal inactive layer, and the detector input window. All dimensions can be entered in "mm", "cm" or "inch" units. In addition to the crystal length and diameter, the dimensions of a cylindrical contact at the rear side of the crystal (a construction feature of conventional coaxial HPGe detectors) can be specified. Up to 6 additional absorbing filters made of Al, Cu, Fe, Pb, Sn, or polyethylene can be placed between source and detector, if one wants to reduce unwanted contribution to the simulated spectrum from the intense low-energy γ -radiation. The user can also add these filters to his virtual spectrometer configuration to simulate γ -spectra from containerized sources. Additional controls for specifying the detector energy resolution properties, number of spectrum channels and channel-to-energy conversion coefficient appear when "Show more settings" checkbox at the bottom right of the measurement setup drawing is selected. Once the user-specific γ -spectrometer is created, it can be saved in user's personal account in NUCLEONICA for future reference and use.

One can start calculations either in an on-line or background mode. In the latter case a notification will be sent via email and a respective alert will be raised in one's NUCLEONICA account, once the task has been completed. There are more settings on the "Options" tab, which provide additional control over the spectrum simulation. For instance, one can enable or disable decay calculations that will or will not allow contributions from decay products, being accumulated during source cooling and spectrum measurement time intervals. The backscatter peak simulation can be also switched on and off, and its contribution to the total detection efficiency can be adjusted using a special scaling factor.

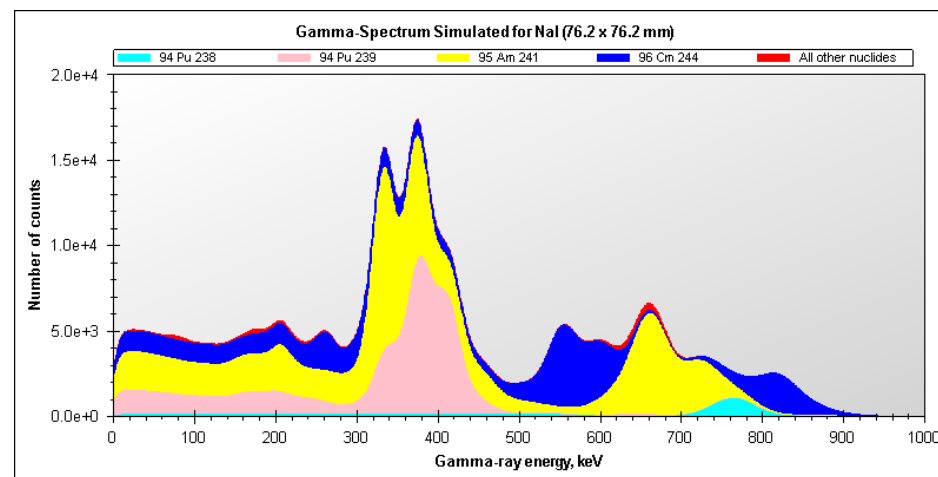
The standard output, which appears in "Calculation results" tab, consists of a stacked graph displaying cumulative and nuclide specific spectra, as well as peak, continuum and backscatter photon contributions to the full spectrum (see Fig.2). One can easily switch between types of spectral information presented on the graph, which include probability density functions for the detector input count rate at start or end of the measurement, as well as mean or statistical (Poisson) number of counts accumulated in spectrum channels. The graph is accompanied by brief numerical information on the total and nuclide specific count rates and number of spectrum counts. Additionally, a graph displaying total detection efficiency for the current spectrometer setup, as well as FEP, SEP, DEP and XEP efficiencies as functions of the incident photon energy can be activated. For both, spectrum and efficiency graphs, a set of controls are provided to tailor their appearance to one's needs and requirements and to download the final image in different graphics formats. A detailed report, containing the complete collection of spectral and efficiency numerical data, is generated also and can be downloaded as a text or Excel spreadsheet file.

4. Some examples

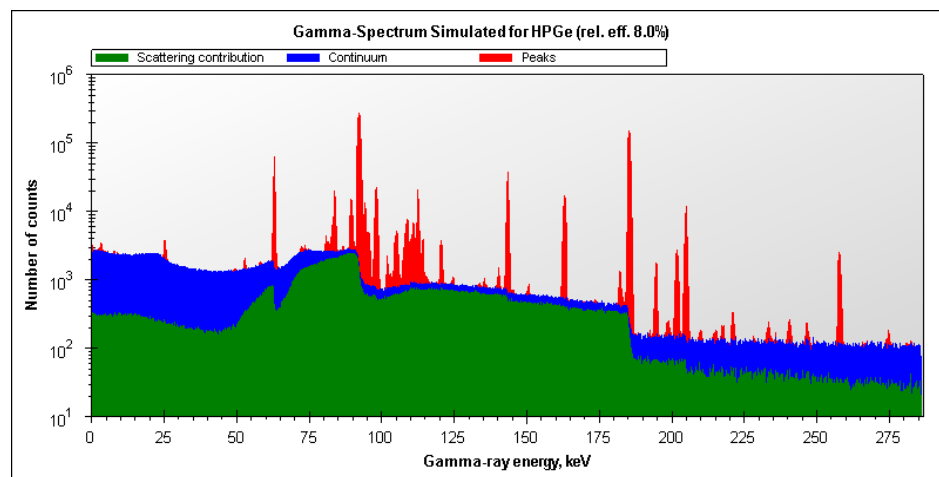
A number of graphs, demonstrating the capabilities of the Gamma Spectrum Generator, are shown in Fig.2. All graphs were created using the generator's tools and downloaded directly from its web-page.



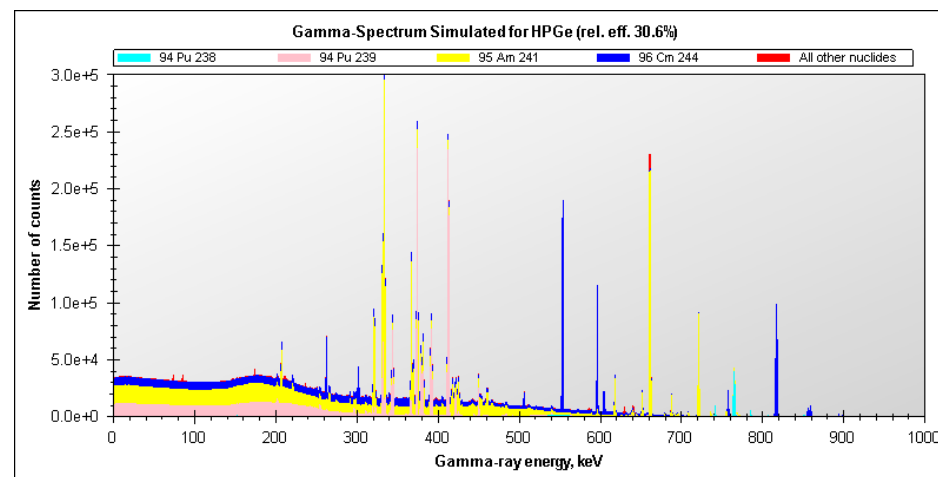
(a)



(c)



(b)



(d)

Fig 3. γ -spectra simulated for: (a) ^{60}Co 100 kBq source and NaI ($\varnothing 3'' \times 3''$) detector, (b) 1 g natural U sample shielded with 0.5 mm Sn and LEGe (20 mm \times 2800 mm²) detector, (c) actinides in 1 kg PWR spent fuel shielded with 5 mm Pb and NaI ($\varnothing 3'' \times 3''$) detector, and (d) actinides in 1 kg PWR spent fuel shielded with 5 mm Pb and BEGe (30% rel. eff.) detector.

Fig.2a shows γ -spectrum simulated for a 100 kBq ^{60}Co source and NaI ($\varnothing 3'' \times 3''$) detector. The source is assumed to be positioned at 25 cm distance from the detector and measured for 1000 s. The graph demonstrates a powerful feature of the generator, which allows to visualize peak and continuum components of the spectrum. In addition, a backscatter peak contribution is shown as a separate continuum component in the graph.

The backscatter photon contribution looks more complicated in the γ -spectrum in Fig.2b. The spectrum was simulated for a 1 g U sample located at 2.5 cm distance from LEGe detector (crystal length 20 mm, active area 2800 mm²) and shielded with 0.5 mm Sn filter. It was assumed that U had been separated from the ore 2 years before the measurement and had natural abundances of ^{234}U , ^{235}U and ^{238}U at the date of the separation. The spectrum includes contributions from all decay products, which have been accumulated since this date. To obtain better statistics of counts, the spectrum measurement time was 10⁵ s.

Fig.2c and Fig.2d show low- and high-resolution γ -spectra for a 5.25 TBq source, which represents actinides extracted from a 1 kg sample of 6-year-aged PWR spent fuel. The isotopic composition of the fuel was calculated using NUCLEONICA's webKORIGEN [4], assuming 4.2% for the original enrichment and 50 GWd/t for the final burnup of the fuel. The low- and high-resolution spectra correspond to NaI ($\varnothing 3'' \times 3''$) and BEGe (30% rel. eff.) detectors, respectively. In both cases the source was assumed to be shielded with a 5 mm Pb filter and located at 25 cm distance from the detectors. The measurement time is 1000 s. From the spectra shown one can see easily the advantages of the high-resolution γ -spectrometry when accurate characterization of the sample is required.

5. Future work

The capabilities of the Gamma Spectrum Generator are planned to be further extended to include simulation of the spectrum distortion effects (e.g. due to coincidence summing and energy resolution deterioration), which may appear in measurements involving elevated count rates and small source-to-detector distances. It is also foreseen to extent the detector response profile database to include LaBr₃ scintillators that, because of their much superior energy resolution, start to replace traditional NaI crystals in many applications. Inclusion of self-attenuation effects is another challenging task, which would allow more realistic simulation of γ -spectra from voluminous sources.

6. Conclusions

A versatile web-accessible γ -spectrum simulation tool has been developed to allow generation of accurate γ -spectra for a wide range of NaI and HPGe detectors and for any mixture of known γ -emitting radionuclides. The simulator is a useful visual teaching aid in providing basic and advanced training for members of nuclear and non-nuclear communities working in various areas of science and technology. The simulator tool is especially useful in training facilities, which have restrictions on the use of radioactive substances, or when sources of special interest (e.g. spent fuel, enriched U, weapon grade Pu or other highly radiotoxic materials) are not readily available.

7. References

- [1] J. Magill et al., NUCLEONICA: A Nuclear Science Portal, ENS News, Issue No.17 Summer (July 2007), see www.euronuclear.org/e-news/e-news-17/nucleonica.htm
- [2] A.N. Berlizov et al., NAAPRO Detector Model, a Versatile and Efficient Approach to γ -ray Spectrum Simulation, Nucl. Instrum. Meth. Phys. Res. A, 562 (2006) 245-253.
- [3] K. Skrable et al., A General Equation for the Kinetics of Linear First Order Phenomena and Suggested Applications, Health Physics, 27 (1974) 155-157.
- [4] A. Schwenk-Ferrero et al., webKORIGEN: Web-based Fuel Cycle Calculations within NUCLEONICA, see <http://www.nucleonica.net:81/wiki/index.php/Help:WebKORIGEN>